

TITLE: New pyrimidine derivatives  
 INVENTOR(S): Boon, Wm. R.; Jones, Wm. G. M.  
 PATENT ASSIGNEE(S): Imperial Chemical Industries Ltd.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	GB 635582		19500412	GB 1947-15606	19470613 ---
AB	<p>5-Nitropyrimidines containing in the 4- or 6-position a ketonylamino or aldehydoamino group are obtained from the 4- or 6-halo analog and the corresponding amino ketone or aldehyde; the NO<sub>2</sub> group may be reduced for continuation of the reaction, which then yields 7,8-dihydropteridines (C.A. numbering). 2,6-Dichloro-5-nitro-4-methylpyrimidine 5 in Me<sub>2</sub>CO 50 and NaHCO<sub>3</sub> 6 treated over 1.5 hrs. with AcCH<sub>2</sub>NH<sub>2</sub> 3 parts yield after filtration and evaporation 2-chloro-4-methyl-5-nitro-6- (acetonylamino)pyrimidine (I), m. 108° (from Et<sub>2</sub>O, EtOAc, and petr. ether). Likewise, I 9 and Et<sub>2</sub>NH 5 parts after 12 hrs. in dioxane yield the 2-diethylamino compound, m. 117-18°, which with H over Raney Ni yields 2-diethylamino-4,6-dimethyl-7,8-dihydropteridine, m. 119-21° (from petr. ether). Similarly, 2,6-dichloro-5-nitropyrimidine in Me<sub>2</sub>CO and NaHCO<sub>3</sub> with AcCH<sub>2</sub>NH<sub>2</sub>.HCl (II) yield 2-chloro-5-nitro-6- (acetonylamino)pyrimidine (III), m. 129-31° (from petr. ether), which in the cold with Et<sub>2</sub>NH in dioxane 12 hrs. yields on dilution with H<sub>2</sub>O 2-diethylamino-5-nitro-6- (acetonylamino)pyrimidine, m. 119° (from EtOAc and petr. ether), while a similar reaction with PhCH<sub>2</sub>NH<sub>2</sub> gave the 2-benzylamino analog, m. 162°. The Et<sub>2</sub>N derivative over Raney Ni in dioxane gave 2-diethylamino-6-methyl-7,8-dihydropteridine, m. 158° (from MeOH). Similarly, 2-methyl-4,6-dichloro-5-nitropyrimidine and II in Me<sub>2</sub>CO in the presence of NaHCO<sub>3</sub> gave 2-methyl-4-chloro-5-nitro-6- (acetonylamino) pyrimidine, m. 84° (from Et<sub>2</sub>O-petr. ether). III 10 in dioxane 50 let stand with 8% NH<sub>4</sub>OH 30 parts gave 2-amino-5-nitro-6- (acetonylamino)pyrimidine, m. 214° (from dioxane), hydrogenated in OHCNMe<sub>2</sub> over Raney Ni to 2-amino-6-methyl-7,8-dihydropteridine, decompose above 210°. 2,6-Dichloro-5-nitropyrimidine (IV) 10 and PhCOCH<sub>2</sub>NH<sub>2</sub>.HCl 11 parts in Et<sub>2</sub>O with NaHCO<sub>3</sub>-H<sub>2</sub>O gave 2-chloro-5-nitro-6- (phenacylamino)pyrimidine, m. 173° (from EtOAc-petr. ether), which with PhCH<sub>2</sub>NH<sub>2</sub> in dioxane gave the 2-benzylamino analog, m. 189° (from dioxane), hydrogenated to 2-benzylamino-6-phenyl-7,8- dihydropteridine, m. pyrimidine 242° (from dioxane). Similar reaction in the cold of IV and AcCHMeNH<sub>2</sub>.HCl in Me<sub>2</sub>CO with NaHCO<sub>3</sub> gave 2-chloro-5-nitro-6-(1-acetyethylamino)pyrimidine, m. 101-2° (from EtOAc-petr. ether); H<sub>2</sub>NCH<sub>2</sub>CH(OEt)2 in the above reaction gave 2-chloro-5-nitro-6-(2,2-diethoxyethylamino)pyrimidine, oil, which allowed to stand 3 hrs. with Et<sub>2</sub>NH in dioxane gave 2-diethylamino-5-nitro-6-(2,2- diethoxyethylamino)pyrimidine, m. 50° (from EtOH); a similar reaction with H<sub>2</sub>NCH<sub>2</sub>CH(SET)2 gave 2-chloro-5-nitro-6-[2,2- bis(ethylmercapto)ethylamino]pyrimidine, oil, which with 10% alc. NH<sub>3</sub> yielded 2-amino-5-nitro-6-[2,2- bis(ethylmercapto)ethylamino]pyrimidine, m. 169° (from EtOH). 4,6-Dichloro-5-nitropyrimidine 4.9 in Me<sub>2</sub>CO 45 containing NaHCO<sub>3</sub> 6.3 and Na<sub>2</sub>S<sub>2</sub>O<sub>4</sub> 5 treated with II 2.8 parts over 0.5 hr. and stirred g hrs. gave 4-chloro-5-nitro-6- (acetonylamino)pyrimidine, m. 60-1° (from petr. ether); the starting material, made from the 4,6-di-HO analog by nitration, followed by treatment with POC1<sub>3</sub>, m. 101-2°.</p>				
IT	875819-80-00P				
	<p>pyrimidinylamino)-          RL: PREP (Preparation)          (preparation of)</p>				
RN	875819-80-0		ZCAPLUS		

CN Acetophenone, 2-(2-benzylamino-5-nitro-4-pyrimidinylamino)- (5CI) (CA  
INDEX NAME)

